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Analysis of Barium Hydroxide and Calcium Hydroxide Slurry Carbonation Reactors

K. D. Patch
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**ANALYSIS OF BARIUM HYDROXIDE AND CALCIUM
HYDROXIDE SLURRY CARBONATION REACTORS**

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ABSTRACT

The removal of CO_2 from air was investigated by using a continuous-agitated-slurry carbonation reactor containing either barium hydroxide $[\text{Ba}(\text{OH})_2]$ or calcium hydroxide $[\text{Ca}(\text{OH})_2]$. Such a process would be applied to scrub $^{14}\text{CO}_2$ from stack gases at nuclear-fuel reprocessing plants. Decontamination factors were characterized for reactor conditions which could alter hydrodynamic behavior. An attempt was made to characterize reactor performance with models assuming both plug flow and various degrees of backmixing in the gas phase. The $\text{Ba}(\text{OH})_2$ slurry enabled increased conversion, but apparently the process was controlled under some conditions by phenomena differing from those observed for carbonation by $\text{Ca}(\text{OH})_2$. Overall reaction mechanisms are postulated.

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1. SUMMARY

Removal of CO_2 (330 ppm) from an air stream was studied in a continuously sparged, agitated-slurry carbonation reactor. The CO_2 content of the outlet gas was measured for barium hydroxide $[\text{Ba}(\text{OH})_2]$ and calcium hydroxide $[\text{Ca}(\text{OH})_2]$ slurries at various operating conditions, and results were compared with those of Sheppard et al. (15), who investigated $\text{Ca}(\text{OH})_2$ slurries. Decontamination factors (DF's) ranged from 3 to 1200 for $\text{Ca}(\text{OH})_2$ and from 60 to 2100 for $\text{Ba}(\text{OH})_2$. For both slurries, lower values of DF were observed at higher gas flow rates and lower impeller speeds. On the other hand, the importance of backmixing for the high-conversion $\text{Ba}(\text{OH})_2$ system apparently caused the DF's to pass through an optimum at conditions toward the opposite extreme, whereas backmixing had a smaller effect on conversion by $\text{Ca}(\text{OH})_2$, which was primarily controlled by the available gas-liquid interfacial area. Increased slurry loadings enhanced conversion for $\text{Ba}(\text{OH})_2$ slurries, in contrast to the opposite effect noted for $\text{Ca}(\text{OH})_2$ slurries. A gas-solid reaction which competes with reactions in the liquid phase is postulated for the $\text{Ba}(\text{OH})_2$ case.

An empirical relationship was developed for the $\text{Ca}(\text{OH})_2$ system, which accounts for a degree of backmixing of the gas phase intermediate to that inherent in the plug-flow and perfectly backmixed models. A nonlinear regression yielded the optimal correlations:

$$a = (7.8 \times 10^{-3}) N^{0.97} U^{0.13} S^{-0.12} d_I^{1.1} \text{ cm}^2/\text{cm}^3$$

$$n = (1.4 \times 10^4) N^{-0.54} U^{0.34} S^{-0.43} d_I^{-3.0}$$

where a is the gas-liquid interfacial area (cm^2/cm^3), n is the number of equal CSTR's (constant stirred tank reactors) in series, N is the impeller speed (rps), U is the superficial gas velocity (cm/s), S is the weight fraction of solids, and d_I is the impeller diameter (cm). Predicted values for interfacial area varied from 0.8 to $2.3 \text{ cm}^2/\text{cm}^3$, and values for the number of equal-volume CSTR's were between 3 and 15. No correlation was recommended for the $\text{Ba}(\text{OH})_2$ system due to the lack of data obtained, the unrealistic values achieved for a and n , and the differing hydrodynamic and chemical phenomena postulated.

2. INTRODUCTION

2.1 Background

Nuclear-fuel reprocessing plants emit stack gases that contain significant amounts of carbon-14 in the form of $^{14}\text{CO}_2$, which should be removed to prevent possible health hazards (5, 6). Carbon-14 has a 5730-yr half-life,

and there is some concern that it may be incorporated into the food chain, possibly leading to mutagenesis. Essentially complete removal of CO_2 from the gas stream can be accomplished by reaction with agitated alkaline slurries. The carbonate product is very stable and satisfies many long-term disposal requirements.

Agitation increases gas-liquid phase subdivision, as well as the degree of liquid-phase mixing. Phase subdivision produces relative motion between the phases and increases the gas-liquid interfacial area (2, 3, 16, 17); both effects contribute to a higher reaction rate by increasing the overall mass transfer. The interfacial area is the principle variable determining the capacity of an agitated gas-liquid reactor (21).

Previous workers (3, 4, 5, 6, 8, 12, 15) have investigated calcium hydroxide $[\text{Ca}(\text{OH})_2]$ slurries for removal of CO_2 . The carbonation reaction for barium hydroxide $[\text{Ba}(\text{OH})_2]$, however, has not been investigated. Studying the significantly higher rate of reaction of $\text{Ba}(\text{OH})_2$, due to the much greater solubility of the hydroxide (5.6 g/100 g H_2O vs 0.2 g/100 g H_2O), should yield a better understanding of the overall carbonation process under slurry conditions.

The objective of this study was to develop a model for the performance of $\text{Ca}(\text{OH})_2$ and $\text{Ba}(\text{OH})_2$ slurry reactors by: (1) developing empirical relationships for interfacial area and degree of mixing as a function of the hydrodynamic parameters of the reactor and (2) summarizing the results from both alkaline slurries to develop a model that can be extended to other systems.

2.2 Theoretical Considerations

2.2.1 Overview

Juvekar and Sharma (8) discuss the overall process for the absorption of CO_2 into an alkaline slurry as outlined below:

where $X = \text{Ba, Ca}$

Reactions (4) and (5) are instantaneous, and thus the rate-controlling step is either the dissolution of the hydroxide or the absorption and subsequent reaction of CO_2 . Reaction (1) is essentially at equilibrium due to the excess of $\text{X(OH)}_2(\text{s})$ present and the relatively small amount of CO_2 absorbed from the gas. Combining the individual rate expressions for the transport of CO_2 through the gas film, transport of CO_2 into the liquid, and reaction of CO_2 with the hydroxyl ions yields the following rate expression (see Appendix 8.1):

$$R_a = K_1 a P_{\text{avg}} x \quad (6)$$

where

R = specific rate of CO_2 absorption (gmol/s-cm^2)

a = gas-liquid interfacial area (cm^2/cm^3)

K_1 = psueo first-order rate constant ($\text{gmol/cm}^2\text{-s-kPa}$)

P_{avg} = average pressure of the gas in the contactor (kPa)

x = mole fraction of CO_2 in the gas

The pseudo first-order rate constant in Eq. (6) is actually a function of several parameters, as given by Danckwerts' surface renewal theory (3):

$$K_1 = \frac{H \sqrt{D_{\text{CO}_2} K_2 [\text{OH}^-] + K_L^2}}{1 + \frac{H \sqrt{D_{\text{CO}_2} K_2 [\text{OH}^-] + K_L^2}}{K_G}} \quad (7)$$

where

D_{CO_2} = diffusivity of CO_2 in aqueous solution (cm^2/s)

H = Henry's coefficient of solubility ($\text{gmol/cm}^3\text{-kPa}$)

K_2 = second-order rate constant ($\text{cm}^3/\text{gmol-s}$)

K_G = gas-side mass transfer coefficient ($\text{gmol/cm}^2\text{-s-kPa}$)

K_L = liquid-side mass transfer coefficient in the absence of chemical reaction (cm/s)

Several authors (7, 8, 15) consider the liquid-phase mass transfer coefficient to be essentially independent of the operating conditions such as gas flow rate, bubble diameter, and mixing intensity; however, there are conflicting opinions concerning this parameter. Danckwerts (3) reports that K_L is constant at relatively low speeds of agitation for which the mean bubble diameter is greater than 2.5 mm. His values for K_L then drop sharply as the speed of agitation is increased and thereafter remain constant. He contends that K_L decreases because bubbles behave hydrodynamically as rigid spheres, with a relatively low K_L , when they are reduced to diameters less than 2.5 mm. Miller (11) also reports that liquid-film-controlled mass transfer is dependent on mean bubble size. Bubble shape, motion, and any tendency for the interface to ripple, fluctuate, or otherwise deform, might also influence mass transfer. Very little information is available in the literature on the gas-side mass transfer coefficient, K_G , in mechanically agitated vessels (10).

Many conflicting investigations of interfacial area have been published in the literature (21). Reith (14) notes that experiments performed in vessels with the same dimensions, filled with the same liquid, and operated under identical conditions, may lead to completely different interfacial areas when different measuring methods (such as light scattering, light reflection, and photography) are used. Calderbank (2), by utilizing a light-scattering technique, showed that the interfacial area across a particular radius of a 100-liter tank can vary from 0.7 to 1.08 cm²/cm³. In addition, extreme variations with reactor depth (0 to 1.2 cm²/cm³) are possible.

The expression most commonly cited for interfacial areas is that derived by Calderbank (2), who correlates interfacial area with the power dissipated by the agitator:

$$a = 1.44 \frac{P^{0.4} \rho^{0.2}}{\sigma^{0.6}} \left(\frac{U}{U_t} \right)^{1/2} \quad (8)$$

$$[(d_I^2 N \rho / \mu)^{0.7} (N d_I / U)^{0/3} < 20,000]$$

where

P = power dissipated per unit volume of liquid (hp/ft³)

ρ = density of the liquid (g/cm³)

σ = surface tension of the liquid (10⁻⁵ J/cm³)

U = superficial gas velocity (cm/s)

U_t = upward velocity of bubbles (typically 26.5 cm/s)

d_I = impeller diameter (cm)

N = frequency of impeller rotation (s^{-1})

μ = liquid viscosity (g/cm-s)

Because Eq. (8) refers to pure liquids rather than to a mixed phase, its usefulness in predicting interfacial areas in slurries is questionable. In addition, the Calderbank correlation relies on an accurate estimate of the power consumption which, for bubbling reactors, requires much empiricism. The complexity of factors influencing power consumption in this case have led some researchers to doubt the practicality of achieving universal relationships to predict power consumption accurately, except for the cases of limited ranges of the relevant variables (18).

2.2.2 Integration of the Carbonation Rate Expression

Equation (6) can be integrated assuming: (1) $K_L a$ is constant throughout the vessel, (2) the liquid is mixed well, and (3) the gas phase is in plug flow. It can then be shown that (see Appendix 8.1):

$$\ln(DF) = \alpha a \quad (9)$$

where

DF = decontamination factor = inlet CO_2 mole fraction/outlet CO_2 mole fraction

$$\alpha = \frac{0.06K_L P_{avg} V_a MW_{air}}{Q \rho_{air}}, \text{ cm}$$

V_a = aerated liquid volume (cm^3)

MW_{air} = molecular weight of air (g/gmol)

Q = air flow rate at 21°C and 101 kPa (L/min)

ρ_{air} = density of air at 21°C and 101 kPa (g/cm^3)

Equation (6) can also be integrated after assuming that the gas phase can be modeled as n equal-volume CSTR's in series, which accounts for varying degrees of backmixing in the gas phase (see Appendix 8.1):

$$DF = \left(1 + \frac{\alpha a}{n}\right)^n \quad (10)$$

If n is unity, Eq. (10) models the behavior of the gas phase as being perfectly backmixed. The limiting behavior as n approaches infinity is that of plug flow, as given by Eq. (9).

3. APPARATUS AND PROCEDURE

3.1 Apparatus

The experimental apparatus is shown in Fig. 1, and vessel specifications are listed in Table 1. The impeller, a 6-bladed Rushton turbine, was driven through a 2:1 reduction gearbox by a compressed-air motor, while the speed was monitored with a stroboscope. Water flowing through cooling coils kept the temperature of the slurry at 292 K.

Table 1. Vessel Specifications

Tank	diameter	27.3 cm
	height	35.0 cm
Baffles	number	4
	width	2.7 cm (1/10 tank diameter)
Impeller	type	6-blade Rushton turbine
	diameter	13.7 cm
	position (above tank bottom)	11 cm (4/10 tank diameter)
Sparger	type	0.95 cm open pipe
	extension above tank bottom	5.5 cm

The reactor was operated in semi-batch mode by continuously passing gas through a slurry. The air flow was measured by a calibrated rotameter and entered the reactor through an open-pipe sparger located directly under the impeller. In all experiments the pressure above the slurry was held at 112 kPa.

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EXPERIMENTAL APPARATUS

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The sample stream of effluent gas passed through a series of three knockout bottles to remove any entrained slurry or condensed water vapor. A bellows pump maintained a constant flow to a Wilkes-Foxboro Model 1-A Infrared Spectrometer set at a wavelength of 4260 nm. Exit CO_2 concentrations were measured at a path length of 20.75 m, with the temperature and pressure kept at 320 K and 136 kPa respectively. The output was displayed on both a digital voltmeter and a strip-chart recorder. A calibration curve allowed conversion of measured voltages to CO_2 concentrations.

3.2 Procedure

The reactor was charged with about 16 liters of slurry containing the desired $\text{Ba}(\text{OH})_2$ solids concentration. The desired air (330 ppm CO_2) flow rate was set, followed by the adjustment of the impeller speed. The exit CO_2 concentration was continuously monitored on the strip-chart recorder, and on reaching steady-state conditions, the agitated slurry height and exit CO_2 concentration were recorded. Care was taken to avoid any entrainment of slurry from the reactor; thus upper limits on the flow rate and impeller speed were established. The values of operating conditions are presented in Table 2.

Table 2. Experimental Variables

Variable	Values
Impeller speed (rpm)	350, 450, 550, 650
Flow rate (l/min)	10, 22, 44
Weight % solids	12, 21
Slurry	$\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$

4. RESULTS AND DISCUSSION

4.1 $\text{Ca}(\text{OH})_2$ Reactor

Preliminary experiments conducted with $\text{Ba}(\text{OH})_2$ slurries indicated severe blockage of the T-sparger located beneath the impeller. It was postulated that the increased rate of reaction, as compared with the $\text{Ca}(\text{OH})_2$ system, resulted in deposition of the carbonate onto the sparger. To circumvent this problem, the T-sparger was removed, leaving an open-pipe sparger. Experiments with $\text{Ca}(\text{OH})_2$ slurries were repeated and compared with results obtained previously (15) (Fig. 2).

Temperature = 292 K

CO₂ Inlet Concentration = 330 ppm

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EXIT CO₂ CONCENTRATION VS IMPELLER SPEED
7 WT % CA(OH)₂ SLURRY

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Westerterp (20) also found that the method of gas injection made little difference if gas were fed to the eye of the impeller. The results shown in Fig. 2 corroborate his observation, with the exception of the open-sparger run at a gas flow rate of 44 l/min. The inconsistently high exit CO_2 concentration at this higher flow rate could be due to some by-passing of large gas bubbles around the impeller. The T-sparger previously used was placed 7.6 cm from the bottom of the tank, whereas the current open-pipe arrangement released the air 5.5 cm from the tank bottom. This effect should be investigated further if more tests are to be run at high gas flow rates with the current sparger arrangement.

The decontamination factors calculated from Fig. 2 range from about 3 to 1200. For both modes of gas introduction, the same qualitative behavior is observed. Extent of reactor conversion increases with increasing impeller speed, but decreases with increasing gas flow rates. Increased agitation is expected to increase the gas-liquid interfacial area because bubbles will rupture and form ones of smaller diameter. This will enhance the extent of conversion if the overall reaction is controlled by mass transfer at the interface and if the increased backmixing associated with greater agitation produces a less significant effect.

Increasing gas flow rate will increase both the mean bubble diameter and the gas holdup (11). The former effect will decrease the specific interfacial area whereas the latter will increase it, so that the overall reactor conversion is not obvious. In addition, greater gas flow rates also lead to shorter residence times and consequently to lower degrees of backmixing, which would tend to enhance reactor conversion. The results in Fig. 2 indicate that the change in mean bubble diameter is the dominating phenomenon under the conditions examined. For the purposes of hydrodynamic modeling, it generally appears that backmixing of the gas phase can be neglected as a first approximation.

By assuming the gas phase to be in plug flow, multiple linear regression techniques were used to obtain the following correlation for interfacial area from the data in Fig. 2 and the additional data of Sheppard *et al.* (15) for $\text{Ca}(\text{OH})_2$ slurries (see Appendix 8.3):

$$a = 0.059 N^{0.63} U^{0.42} S^{-0.116} d_I^{0.44} \text{ cm}^2/\text{cm}^3 \quad (11)$$

where N is the impeller speed (rps), U is the superficial gas velocity (cm/s), S is the weight fraction of solids, and d_I is the impeller diameter (cm). The correlation predicts the interfacial area will increase with increasing impeller speed and gas flow rate, as was postulated above. Calculated interfacial areas ranged from 0.5 to 2.0 cm^2/cm^3 , results which are within the range of reasonable values (8, 14, 21). Interfacial areas were also calculated when assuming a backmixed gas phase but those values, ranging from 1.5 to 150 cm^2/cm^3 , seemed to be excessively large (see Appendix 8.3).

Many authors feel that the gas phase is best described by plug flow (7, 11, 12) especially at low speeds of agitation; however, there are

conflicting opinions as to whether a plug flow or backmixed model is appropriate. Calderbank (2) finds that his results correlate best when complete backmixing is assumed. Several authors (11, 18, 19) find that impeller-induced coalescence of recirculating bubbles is significant and, under many conditions, the gas bubbles leaving the impeller zone are composed mainly of recirculating gas. In addition, it has been demonstrated that gas bubbles passing through the impeller region are much more likely to be coalesced in pockets above the impeller blades than to undergo simple rupturing that has been previously envisaged (19). Thus, neither a simple plug-flow nor a perfectly backmixed model for the gas phase can be considered adequate.

The experimental data also exhibit the inadequacy of a plug-flow model. A comparison of measured decontamination factors with those predicted by the plug-flow model is presented in Fig. 3. Although the correlation seems to be acceptable at lower decontamination factors, reactor efficiency is overestimated at conditions producing higher decontamination factors. Backmixing appears to significantly reduce the conversion efficiency if the reactor is operated at low flow rates and high impeller speeds.

In an attempt to account for different degrees of backmixing in the gas phase, the system was modeled as CSTR's in series. Simultaneous empirical relationships were obtained for the number of equal-volume CSTR's n and the interfacial areas a as functions of the measured hydrodynamic parameters of the reactor. Using nonlinear regression (see Appendix 3.1), power-law correlations of the following form result

$$n = (1.4 \times 10^4) N^{-0.54} U^{0.34} S^{-0.43} d_I^{-3.0} \quad (12)$$

$$a = (7.8 \times 10^{-3}) N^{0.97} U^{0.13} S^{-0.11} d_I^{1.1} \quad (13)$$

The model predicts an increase in interfacial area with increases in impeller speed, gas flow rate, and impeller diameter, as expected. A decrease in interfacial area is indicated for an increase in solids content, possibly due to bubble coalescence at the solid particles. A trend toward greater backmixing (decreasing n) occurs with increasing impeller speed, impeller diameter, and solids content, whereas an increase in gas flow rate suggests an approach to plug-flow conditions. Values of interfacial area generated from this model range from 0.8 to 2.3 cm²/cm³, and the number of equal-volume CSTR's varies between 3 and 15. Values of n greater than 10 can be shown to indicate essentially plug-flow behavior (9).

A measure of the applicability of this model is shown in Fig. 4, where measured and predicted decontamination factors are compared. In contrast to Fig. 3, the correlation appears to be an improved representation of the experimental data throughout the range studied.

Temperature = 292 K

x = mole fraction CO_2

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PREDICTED VS EXPERIMENTAL
DECONTAMINATION FACTORS
FOR PLUG-FLOW MODEL

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4.2 Ba(OH)₂ Reactor

Initial studies involving Ba(OH)₂ indicated that foaming of the slurry was a significant problem which led to the entrainment and deposition of slurry in the sample line and the first knockout pot. The gas flow rates examined were consequently restricted to values less than 50 l/min.

The Ba(OH)₂ slurries yielded substantially higher conversions than did the Ca(OH)₂ cases investigated. From Figs. 5 and 6, decontamination factors for the former can be calculated as ranging from 60 to 2100. The different qualitative behavior of these curves also suggests the possibility of other overall reaction mechanisms under these conditions.

Figure 5 illustrates the effect of flow rate on exit CO₂ concentration as a function of impeller speed. Note that exit CO₂ concentrations are an order of magnitude less than those obtained for Ca(OH)₂ (Fig. 2). The Ba(OH)₂ curves reach a CO₂ concentration minimum at approximately 550 rpm, in contrast to the Ca(OH)₂ slurries, for which the CO₂ concentration steadily decreases with increasing impeller speed (Fig. 2). Apparently the increased backmixing at higher agitation speeds and lower gas flow rates is not balanced by a corresponding increase in interfacial area. Slight changes in the residence-time distribution at the high conversions of the Ba(OH)₂ system (~99.9%) could significantly alter the extent of reactor conversion and lead to the effects observed.

The effect of solids content on CO₂ conversion is shown in Fig. 6. The apparent trend indicates that CO₂ removal efficiency improves with increasing solids content. The Ca(OH)₂ system manifests the opposite effect. The explanation may lie in competing effects between bubble coalescence and gas-solid reaction. As mentioned above (Sect. 4.1), increased solids concentration may increase bubble coalescence and thus decrease interfacial area and conversion; however, it is also possible that a significant gas-solid reaction exists. If the gas-solid reaction effect were more pronounced than the coalescence effect, one would expect the trend observed in Fig. 6. The literature does not elucidate this problem but only states that conversion is highly dependent on the system in question.

From the above discussion and attempted correlations using the experimental data, it is obvious that the simple plug-flow model above could not explain the observed behavior of the Ba(OH)₂ system. In addition, modeling the system as a series of stirred tanks yields results that are physically intractable. Since the optimal correlation predicts 0.1 CSTR in series and interfacial areas on the order of 10^{50} cm²/cm³, the results are clearly unrealistic. Undoubtedly the poor correlation is also attributable to the lack of data; only 27 data points are available for the nonlinear-regression correlation of eight parameters (96 data points are used for the Ca(OH)₂ correlation). Evidently a better knowledge of the residence-time distribution of the gas and the variation of mass transfer coefficients, as functions of the various hydrodynamic parameters, is required to predict the behavior of hydroxide slurry carbonation reactors operating at conversions exceeding 99%.

Temperature = 292 K

x = mole fraction CO_2

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PREDICTED VS EXPERIMENTAL
DECONTAMINATION FACTORS
FOR n CSTR'S IN SERIES MODEL

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FIG.
4

Temperature = 292 K

Inlet concentration of CO₂ = 330 ppm

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EXIT CO₂ CONCENTRATION VS IMPELLER SPEED
FOR 21 WT % Ba(OH)₂ SLURRY

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Temperature = 292 K

Inlet concentration of CO_2 = 330 ppm

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EXIT CO_2 CONCENTRATION VS IMPELLER SPEED
FOR DIFFERENT SOLIDS LOADINGS

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FIG.
6

5. Conclusions

1. $\text{Ba}(\text{OH})_2$ has a much greater CO_2 removal efficiency than $\text{Ca}(\text{OH})_2$.
2. It is possible to model $\text{Ca}(\text{OH})_2$ slurries by accounting for both the interfacial area and degree of mixing as functions of the hydrodynamic parameters.
3. $\text{Ba}(\text{OH})_2$ slurries cannot be characterized by using simple plug-flow or backmixed models.
4. $\text{Ba}(\text{OH})_2$ slurries produce an increase in CO_2 removal efficiency with increasing solids concentration, whereas the opposite behavior is noted for $\text{Ca}(\text{OH})_2$ slurries.

6. Recommendations

1. A better knowledge of residence-time distributions of the gas phase in the agitated contactor is necessary when attempting to correlate interfacial areas in slurry reactors.
2. Additional $\text{Ba}(\text{OH})_2$ data are needed to better characterize system behavior.
3. Relationships for mass transfer coefficients as functions of hydrodynamic parameters of the reactor are needed to improve modeling of slurry systems.
4. Improvements in the reactor design could be made by placing the sparger closer to the impeller to avoid gas bypassing and increasing dead height above the slurry surface to reduce entrainment of $\text{Ba}(\text{OH})_2$ foam.

7. Acknowledgment

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8. APPENDIX

8.1 Carbonation Rate and Interfacial Area Expressions

The rate of reaction of CO_2 in the liquid film is given by Dankwerts' surface renewal theory (3):

$$Ra = K_R a P_I \quad (14)$$

where

$$K_R = H \sqrt{D_{\text{CO}_2} K_2 [\text{OH}^-] + K_L^2}$$

R = specific rate of absorption of CO_2 , $\text{gmol/cm}^3\text{-s}$

a = interfacial area, cm^2/cm^3

H = Henry's coefficient of solubility, $\text{gmol/cm}^3\text{-kPa}$

D_{CO_2} = diffusivity of CO_2 in aqueous solution, cm^2/s

K_2 = second order rate constant, $\text{cm}^3/\text{gmol-s}$

$[\text{OH}^-]$ = hydroxide concentration, gmol/cm^3

K_L = liquid side mass transfer coefficient, cm/s

P_I = partial pressure of CO_2 at the gas/liquid interface, kPa

The rate of reaction in the liquid must be balanced by the rate of transport of CO_2 through the gas film at steady state (8):

$$Ra = K_G a (P_G - P_I) \quad (15)$$

where K_G is the gas side mass transfer coefficient ($\text{gmol/cm}^2\text{-kPa}$) and P_G is the partial pressure of CO_2 in the gas stream (kPa). Eliminating P_I from Eqs. (14) and (15) gives:

$$Ra = \left[\frac{K_R}{1 + (K_R/K_G)} \right] a P_G = K_1 a P_G \quad (16)$$

where K_1 is a pseudo first-order rate constant, $\text{gmol/cm}^2\text{-kPa-s}$. The partial pressure of CO_2 can be related to the total pressure by

$$P_G = x P_{\text{avg}} \quad (17)$$

where x is the mole fraction of CO_2 in the air stream and P_{avg} is the average pressure in the contactor, kPa. Combining Eqs. (16) and (17) we obtain:

$$R_a = K_1 a P_{\text{avg}} x \quad (6)$$

Under the assumptions that the liquid phase is well-mixed and that the gas travels through the contactor in essentially plug flow, we can write the following differential mass balance on CO_2 :

$$-G dx = R_a A dz \quad (18)$$

where G is the molar gas flow rate (gmol/s), A is the contactor cross-sectional area (cm^2), and z is the vertical height in the reactor (cm). Combining Eqs. (6) and (18) and integrating between initial and final conditions yields the equation given previously:

$$\ln\left(\frac{x_0}{x_f}\right) = \alpha a \quad (9)$$

Treating the gas phase as n equal-volume CSTR's in series [as opposed to an infinite number which is implicit in the development of Eq. (9)], one can easily obtain:

$$\frac{x_0}{x_f} = \left(1 + \frac{\alpha a}{n}\right)^n \quad (10)$$

8.2 Physical and Chemical Properties

8.2.1 Henry's Law Constant

At 20°C the solubility of Ba(OH)_2 in water is $5.6 \text{ g/100 g water}$; therefore, the concentration of the OH^- ions is 0.355 M . The Henry's Law solubility constant for CO_2 in pure water (H_2O) at 20°C is $3.9 \times 10^{-7} \text{ gmol/cm}^3\text{-kPa}$ (3). The correction for the effect of ionic strength or Henry's constant is (3):

$$\log\left(\frac{H}{H_0}\right) = -h I \quad (19)$$

where h is the sum of contributions referring to the species of positive and negative ions present, and I is the ionic strength of the solution defined as:

$$I = \frac{1}{2} \sum C_i Z_i^2 \quad (20)$$

where C_i is the concentration of ions of valence Z_i . Using these values for h from Danckwerts (4), $h = 0.115$ and $I = 0.532$, and substituting into Eq. (19), H was found to equal 3.4×10^{-7} gmol/cm³-kPa.

8.2.2 Rate Constant (K_2)

The reaction between CO_2 and OH^- is

and the rate expression is

$$R = K_2 [\text{CO}_2] [\text{OH}^-] \quad (22)$$

At infinite dilution the rate constant in pure water K_2^0 is 5900 l/gmol-s at 20°C (4). A correction must be made for the ionic strength of the solution, using Fig. 6 in Danckwerts and Sharma (4):

$$K_2 = K_2^0 + 3200 I \quad (23)$$

where I is the ionic strength. Therefore, the corrected rate constants are:

$$\text{Ba(OH)}_2: K_2 = 7600 \text{ l/gmol}$$

$$\text{Ca(OH)}_2: K_2 = 6050 \text{ l/gmol}$$

8.2.3 Diffusivity

The diffusivity of CO_2 in water at 20°C when the viscosity is 1.1×10^{-2} g/cm-s was found to be (13):

$$D_{\text{CO}_2} = 1.4 \times 10^{-5} \text{ cm}^2/\text{s}$$

8.2.4 Mass Transfer Coefficients

The liquid-side mass transfer coefficient for CO_2 , K_L , was estimated by Juvekar and Sharma (7) to be:

$$K_L = 6.5 \times 10^{-2} \text{ cm/s}$$

This value was constant over the range of experimental conditions considered. The gas-side mass transfer coefficient for CO_2 , K_G , was estimated from measured values of $K_G a$, where a is the interfacial area. Values of this product are approximately 10^{-6} gmol/cm³-s-kPa (7). If the interfacial area is assumed to be $2 \text{ cm}^2/\text{cm}^3$, the value of K_G is about 5×10^{-7} gmol/cm²-kPa-s.

8.2.5 Viscosity and Density

The slurry densities were measured by making up the appropriate solution volumetrically and weighing the solution. Viscosities at 20°C were measured with a Brookfield viscometer fitted with an Ultra-viscosity spindle which rotated at 60 rpm. The results are shown in Table 3.

Table 3. Viscosities and Densities

Solution	% Solids	Density (g/cm ³)	Viscosity (10^{-2} g/cm-s)
0.5 M $\text{Ca}(\text{OH})_2$	3.64	1.018	1.099
1.0 M $\text{Ca}(\text{OH})_2$	7.14	1.038	1.210
1.5 M $\text{Ca}(\text{OH})_2$	10.56	1.056	1.484
0.4 M $\text{Ba}(\text{OH})_2$	11.86	1.064	1.150
0.75 M $\text{Ba}(\text{OH})_2$	21.11	1.121	1.200

8.3 Data and Computer Analysis

Three computer programs were written to analyze the data. Two were statistical analyses programs, while the third placed the data into a form convenient for analysis. The first program listed was the program used to calculate interfacial areas and decontamination factors (DF). Data were read in free format from a data file, in this case FOR21.DAT. Calculations of interfacial area and DF were stored along with the initial data in a new data file, FOR22.DAT, which was compatible with the statistical programs. Separate versions of the program were made for the barium hydroxide data, the 1979 calcium hydroxide data from this study, and the calcium hydroxide study of Sheppard et al. (15), along with separate sets of data files. The original data and the calculated interfacial areas obtained by using ideal reactor models are tabulated in Table 4.

The other programs were written to use the Statistical Analysis System (1) package available on the IBM 360 computer at ORNL. The second program listed attempted to correlate interfacial area using a General Linear Models Procedure (GLM). The GLM program used a multiple linear regression to fit the data to the specified model. In addition, a stepwise regression procedure was used to find the collection of independent variables that best fit the data. The third program used a nonlinear regression procedure to fit the data to a n-CSTR's-in-series model. The program produces least-squares estimates of the parameters of the nonlinear model specified.

1. Program 1

TYPE CALCBA.FOR

```

00100  C*** THIS PROGRAM CALCULATES INTERFACIAL AREAS (I.A.'S)
00200  C*** FOR BA(OH)2 SLURRIES BASED UPON TWO MODELS:
00300  C*** 1. PERFECT BACKMIXING ( ONE CSTR)
00400  C*** 2. PERFECT PLUG FLOW
00500  C*** THE THEORETICAL DEVELOPMENT IS DETAILED IN CEPS-X-300
00600  C***
00700  C*** THE VARIABLES USED ARE:
00800  C*** AIRDEN = DENSITY OF AIR (G/CC)
00900  C*** AIRWT = MOLECULAR WEIGHT OF AIR (G/G-MOL)
01000  C*** ALPHA = A RATIO OF REACTION RATE TO GAS
01100  C*** FLOW RATE. (CM)
01200  C*** AMIX = BACKMIXED INTERFACIAL AREA (CM2/CM3)
01300  C*** APLUG = PLUG FLOW INTERFACIAL AREA (CM2/CM3)
01400  C*** C02IN = INLET CO2 CONCENTRATION (PPR)
01500  C*** C02OUT = OUTLET CO2 CONCENTRATION (PPR)
01600  C*** DC02 = DIFFUSIVITY OF CO2 IN AQUEOUS
01700  C*** SOLUTION (CM2/S)
01800  C*** DIMP = IMPELLER DIAMETER (CM)
01900  C*** FLOW = VOLUMETRIC FLOW RATE (L/MIN)
02000  C*** HEIT = AERATED HEIGHT IN CONTACTOR (CM)
02100  C*** HEITC = UNAGITATED SLURRY HEIGHT (CM)
02200  C*** HENRYS = HENRY'S COEFFICIENT OF SOLUBILITY
02300  C*** (G-MOL/CC-ATM)
02350  C*** IDF = DECONTAMINATION FACTOR
02400  C*** IRPM = REVOLUTIONS PER MINUTE OF THE
02500  C*** AGITATOR (/MIN)
02600  C*** IRUN = DATA POINT NUMBER
02700  C*** NPTS = NUMBER OF DATA POINTS
02800  C*** OH = CONCENTRATION OF HYDROXIDE (G-MOL/CC)
02850  C*** PER SOL = PERCENT SOLIDS IN SLURRY SOLUTION
02900  C*** PIN = INLET GAS PRESSURE (PSIG)
03000  C*** PAV = AVERAGE GAS PRESSURE IN REACTOR (ATM)
03100  C*** S = CROSS-SECTIONAL AREA OF CONTACTOR (CM2)
03200  C*** SLURRY = SLURRY "PSEUDO MOLARITY" (MOL/L)
03300  C*** VA = AERATED VOLUME (CC)
03350  C*** VISC = VISCOSITY OF SLURRY SOLUTION (CP)
03400  C*** XKG = GAS SIDE MASS TRANSFER COEFFICIENT
03500  C*** OF CO2 (G-MOL/CM2-S-ATM)
03600  C*** XKL = LIQUID SIDE MASS TRANSFER
03700  C*** COEFFICIENT OF CO2 (CM/S)
03800  C*** XKR = A LUMPED REACTION CONSTANT (G-MOL/CM2-S-ATM)
03900  C*** XK1 = PSEUDO FIRST ORDER RATE CONSTANT
04000  C*** (G-MOL/CM2-S-ATM)
04100  C*** XK2 = SECOND ORDER RATE CONSTANT (CC/G-MOL-S)
04200  C*** DATA AIRDEN/.001205/,AIRWT/28.964/,C02IN/3.3F5/,
04300  C*** IDC02/1.4E-5/,HENRYS/3.40E-5/,OH/3.55E-4/,S/585./,
04400  C*** 2XKG/5.E-5/,XKL/6.5E-2/,XK2/7.6E6/
04500  C*** XKR = HENRYS * SORT( DC02 * XK2 * OH + XKL**2)
04600  C*** XK1 = XKR / (1.0 + XKR/XKG)
04620  C*** NOTE: PRESSURE ABOVE CONTACTOR MAINTAINED AT 1.5 PSIG

```

```

04640 C*** WE ASSUME PRESSURE TO BE DUE TO ONLY THE HYDROSTATIC
04660 C*** HEAD OF WATER IN THE CONTACTOR.
04680 PAV = 1.115
04700 READ ( 21,10) NPTS
04800 10 FORMAT (I)
04900 DO 100 J = 1,NPTS
05000 READ (21,20)IRUN, DIMP, IRPM, SLURY, PIN, FLOW, HEIT,
05100 IHEITC, C02OUT
05200 20 FORMAT (I,F,I,F)
05400 VA = S * HEIT
05500 ALPHA = 0.06 * XKI * PAV * VA * AIRWT/(FLOW * AIRDEN)
05600 C*** CALCULATE INTERFACIAL AREA FOR PLUG FLOW MODEL
05700 APLUG = ALOG(C02IN/C02OUT)/ALPHA
05800 C*** CALCULATE INTERFACIAL AREA FOR BACKMIXED MODEL
05900 AMIX = (C02IN/C02OUT - 1.0)/ALPHA
05930 IF (SLURY .EQ. 0.75) RH0 = 1.121
05960 IF (SLURY .EQ. 0.40) RH0 = 1.064
06000 IF (SLURY .EQ. 0.75) PERSOL = 0.2111
06100 IF (SLURY .EQ. 0.4) PERSOL = 0.1186
06200 IF (SLURY .EQ. 0.75) VISC = 1.200
06300 IF (SLURY .EQ. 0.4) VISC = 1.150
06400 C*** CALCULATE DECONTAMINATION FACTOR
06500 IDF = C02IN/C02OUT + 0.5
06600 C*** STORE DATA IN FOR22.DAT FOR ANALYSIS BY SAS PROGRAM
06700 WRITE(22,30)IRUN, IRPM, FLOW, DIMP, RH0, PERSOL, VISC,
06800 IHEITC, HEIT, IDF, ALPHA, APLUG, AMIX
06900 30 FORMAT(13,14,F5.1,F5.1,F6.3,F6.4,F6.3,2F5.1,15,F8.4,
06950 IF5.2,F7.2)
07000 100 CONTINUE
07100 STOP
07200 END

```

2. Program 2

```

TYPE SAS1.JCL
//RPH1 JOB (16417), 'RIN P, K.D. PATCH'
//*CLASS CPH91=405,PRINT=50,CARDS=99,IO=3
//ROUTE PRINT LOCAL
// EXEC SAS76
//STEPLIB DD DSN=A.F.IN10307.SAS.LIBRARY,DISP=SHR
//SAS.SYSIN DD *
***
THIS PROGRAM CORRELATES HYDRODYNAMIC PARAMETERS WITH
INTERFACIAL AREA AND PLOTS THE RESULTS. IT ALSO
ATTEMPTS TO FIT THE DATA TO THE BEST EMPIRICAL MODEL.
***
THE BULK OF THE PROGRAM CONTAINS MISCELLANEOUS
CORRELATIONS FROM CEPS-X-281 (1978):
DATA IHTFP;
***

```

```

READ VARIABLES FROM DATA FILE:
  EXPERIMENTAL RUN, SPEED (RPM), GASFLOW RATE (L/MIN),
  IMPELLER DIAMETER (CM), RHO (G/CC), FRACTIONAL PERCENT
  SOLIDS IN SLURRY, SLURRY VISCOSITY (CP), UNAGITATED
  SLURRY HEIGHT (CM), AFRATED SLURRY HEIGHT (CM),
  DECONTAMINATION FACTOR, ALPHA (CM), PLUG FLOW INTERFACIAL
  AREA (CM2/CC), BACKMIX INTERFACIAL AREA (CM2/CC);
INPUT RUN 1-3 RPM 4-7 GASFLOW 8-12 IMPDIAM 13-17 RHO 18-23
  PERSOL 24-29 VISC 30-35 OFFHT 36-40 AFRHT 41-45 DF 46-50
  ALPHA 51-58 APLUG 59-63 AMIX 64-70;
AGE = 1;
IF -N- > 96 THEN AGE = 2;
***
WE ARE GOING TO FIT A LINEAR MODEL TO THE EXPERIMENTAL
  DATA USING AN EQUATION OF THE FORM:
  LN(ARFA) = A LN(RPM) + B LN(GASFLOW) ...;
***
CONVERT GAS FLOW RATE TO SUPERFICIAL VELOCITY (CM/S);
FLOW = GASFLOW;
II = GASFLOW * .02849;
***
CALCULATE THE REYNOLDS NUMBER;
REYN=IMPDIAM*IMPDIAM*RPM*RHO/VISC/60;
***
CALCULATE THE FROUDE NUMBER;
FROUDE= IMPDIAM*RPM*RPM/3600/980;
***
CONVERT RPM TO REVOLUTIONS PER SECOND;
RPS=RPM/60;
***
  CREATE A DIMENSIONLESS VARIABLE;
  NDSV = IMPDIAM*RPS/II;
***
TAKE LOGARITHMS OF THE VARIABLES TO BE CORRELATED;
***
IMPELLER SPEED;
LNRPS=LOG(RPS);
***
IMPELLER DIAMETER;
LNDIAM=LOG(IMPDIAM);
***
SUPERFICIAL VELOCITY;
LNQG=LOG(II);
***
INTERFACIAL AREA FOR PLUG FLOW MODEL;
LNAPLUG=LOG(APLUG);
***
INTERFACIAL AREA, BACKMIX ASSUMPTION;
LNAMIX=LOG(AMIX);
***
REYNOLDS NUMBER;
LNRFIN=LOG(REYN);
***
VISCOSITY;
LNVISC=LOG(VISC);
***

```

NEW DIMENSIONLESS VARIABLE;
LNNDSV=LOG(NDSV);

FRUIDE NUMBER;
LNFR= LOG(FRUIDE);

PER CENT SOLIDS;
LNPFERSOL=LOG(PERSOL);

DECONTAMINATION FACTOR;
LNDF = LOG(DF);

READ IN DATA;
CARDS;
=FOR12.DAT;

;

PERFORM THE LINEAR MODELS PROCEDURE;
PROC GLM DATA= INTFP;
MODEL LNDF LNAPLIIG LNAMIX=LNFRPS LNOG LNDIAM LNPFERSOL;
OUTPUT OUT= RESULTS PREDICTED= CDF CAPLIIG CAMIX
RESIDUAL= RDF RPLIIG RMIX;
TITLE PLUGFLOW CORRELATION;

PRINT THE RESULTS;
PROC PRINT;

MAKE SUBSETS OF THE RESULTS FOR PLOTTING;

MAKE PLOTS OF RESULTS;
PROC PLOT DATA = RESULTS;
PLOT LNAPLIIG*CAPLIIG=RPM LNAPLIIG*CAPLIIG=FLOW LNAPLIIG*CAPLIIG=AGE;
TITLE1 PLOT OF LOG INTERFACIAL AREA (PLUG GASFLOW) VS. CORRELATION;
PROC PLOT DATA = RESULTS;
PLOT LNDF*CDF=RPM LNDF*CDF=FLOW LNDF*CDF=AGE;
TITLE1 PLOT OF LOG DECONTAMINATION FACTOR VS. CORRELATION;
PROC PLOT DATA = RESULTS;
PLOT LNAMIX*CAMIX=RPM LNAMIX*CAMIX=FLOW LNAMIX*CAMIX=AGE;
TITLE1 PLOT OF LOG INTERFACIAL AREA (BACKMIX) VS. CORRELATION;
PLOT RDF*RPM=FLOW RPLIIG*RPM=FLOW RMIX*RPM=FLOW;
TITLE1 PLOT OF RESIDUAL VS. RPM BY FLOW RATES;

;

PROC GLM DATA= INTFP;
MODEL LNAPLIIG= LNFR LNNDSV LNPFERSOL/P;
OUTPUT OUT= INT PREDICTED= CAPLIIG RESIDUAL= RESID;
TITLE PLUGFLOW CORRELATION;
PROC PLOT DATA= INT;
PLOT LNAPLIIG*CAPLIIG=RPM;
TITLE1 PLOT OF LOG INTERFACIAL AREA VS. CORRELATION;
TITLE2 INTERCEPT INCLUDED IN CORRELATION;

;

PROC GLM DATA= INTFP;
MODEL LNAPLIIG= LNFRPS LNOG LNPFERSOL LNDIAM/P;
OUTPUT OUT= NOINT PREDICTED= CAPLIIG RESIDUAL= RESID;
TITLE PLUGFLOW CORRELATION;

```

PROC PLOT DATA= N0INT;
  PLOT LNAPLIIG*CAPLIIG=RPM;
  TITLE1 PLOT OF LOG INTERFACIAL AREA VS. CORRELATION;
  TITLE2 INTERCEPT WAS NOT INCLUDED IN CORRELATION;
***
;
PROC GLM DATA= IHTFP;
  MODEL LNAPLIIG= LNRPS LNOG LNPERSOL / N0INT P;
  TITLE PLUGFLOW CORRELATION;
***
;
PROC GLM DATA= IHTFP;
  MODEL LNAPLIIG= LNFR LNRFYN LNNDVS LNPERSOL/P;
  TITLE PLUGFLOW CORRELATION, DIMENSIONLESS VARIABLES;
***
;
PROC GLM DATA= IHTFP;
  MODEL LNAPLIIG= LNREYN LNNDVS LNPERSOL/P;
  TITLE PLUGFLOW CORRELATION, REYNOLDS NO., SUPERFICIAL
  GAS VEL., AND PERCENT SOLIDS.;
***
USE THE STEPWISE PROCEDURE TO FIND THE RES
PROC STEPWISE DATA= IHTFP;
  MODEL LNAPLIIG= LNRPS LNOG LNDIAM LNPERSOL / MAXR;
  MODEL LNAPLIIG= LNRFYN LNFR LNOG / MAXR;
/*
//
ENDINPUT

```

3. Program 3

```

TYPE NLBA..JCL
//VAS3 JOB (16417), 'RIN P, K.D. PATCH'
//*CLASS CPII91=6M,10=2
/*ROUTE PRINT LOCAL
// EXEC SAS76
//STEPLIB DD DSN=A.EJN10307.SAS.LIBRARY,DISP=SHR
//SAS.SYSIN DD *

```

```

***
PROGRAM TO CORRELATE INTERFACIAL AREAS AND
DEGREE OF MIXEDNESS FOR 1979 BA(OH)2 DATA
***

```

VARIABLE	DESCRIPTION	UNITS
A	INTERFACIAL AREA	(CM ² /CM ³)
AIRFLOW	AIR FLOW RATE AT STP	(L/MIN)
ALPHA	A RATIO OF REACTION RATE TO GAS FLOW RATE	(CM)
DF	DECONTAMINATION FACTOR	
HEIT	AGITATED SLURRY HEIGHT	(CM)
IMPDIAM	IMPELLER DIAMETER	(CM)
N	NO. OF CSTR'S IN SERIES	
PERSOL	PERCENT SOLIDS	
RPM	AGITATOR SPEED	(RPM)
RUN	RUN NO.	
U	SUPERFICIAL VELOCITY	(CM/S)


```

***
READ VARIABLES FROM DATA FILE:
DATA:
INPUT RIN 1-3 RIM 4-7 AIRFLOW R-10 IMPDIAM 13-17
PERSOL 24-29 NFIT 41-45 DE 46-50 ALPHA 51-58:
***
USE LN OF DECONTAMINATION FACTOR FOR CORRELATION:
LNDF = LOG(DF):
***
CALCULATE SUPERFICIAL VELOCITY FROM AIRFLOW AND
CONTACTOR CROSS-SECTIONAL AREA (585 CM2):
U = AIRFLOW*0.02849:
***
CONVERT RPM TO KPS:
RPS = RPM/60.0:
CARDS:
=FOR22.DAT:
:
***
TANKS IN SERIES MODEL:
POSTULATE CONTACTOR CAN BE MODELED AS N-CSTR'S
IN SERIES. CORRELATE 'N' AND 'A' AS FUNCTIONS
OF THE HYDRODYNAMIC VARIABLES. :
***
NOTE: THE IMPELLER DIAMETER WAS NOT VARIED AND
IS THEREFORE NOT INCLUDED IN THE MODEL:
PROC NLIN ITER=500 METHOD=PARQUARDT:
PARAMETERS A0=1.8F9
          A1=6.3
          A2=-2.0
          A3=0.952
          N0=0.3225
          N1=-0.859
          N2=-0.225
          N3=-0.14:
BOUNDS A0>0 N0>0:
***
POSTULATE EMPIRICAL RELATIONSHIPS AS FOLLOWS:
A=A0*(RPS**A1)*(U**A2)*(PERSOL**A3):
N=N0*(RPS**N1)*(U**N2)*(PERSOL**N3):
GAMMA = ALPHA*A/N:
GAMMA1 = GAMMA + 1.0:
DFRA = (ALPHA/GAMMA1)**A:
DFRN = (LOG(GAMMA1) - GAMMA/GAMMA1)*N:
MODEL LNDF = N*LOG(GAMMA1):
DFR.A0=DFRA/A0:
DFR.A1=DFRA*LOG(RPS):
DFR.A2=DFRA*LOG(U):
DFR.A3=DFRA*LOG(PERSOL):
DFR.N0=DFRN/N0:
DFR.N1=DFRN*LOG(RPS):
DFR.N2=DFRN*LOG(U):
DFR.N3=DFRN*LOG(PERSOL):
OUPUT OUT=CSTR PREDICTED=LNDF1 RESIDUAL=RESID
PARMS=F1-FR:
DATA RESULTS:
SET CSTR:
AREA=F1*(RPS**F2)*(U**F3)*(PERSOL**F4):
NCSTR=F5*(RPS**F6)*(U**F7)*(PERSOL**F8):
PROC PRINT DATA=RESULTS:
PROC PLOT DATA=RESULTS:
  PLOT LNDF*LNDF1=RPS:
  LABEL LNDF=LOG DECONTAMINATION FACTOR
        LNDF1=LOG DECONTAMINATION FACTOR (PREDICTED):
  TITLE LOG DECONTAMINATION FACTOR ACTUAL VS. PREDICTED:
  TITLE2 N-CSTR'S IN SERIES MODEL 1979 RACON2 DATA:
PROC PLOT DATA=RESULTS:
  PLOT RESID*LNDF1=RPS RESID*LNDF1=AIRFLOW:
/*
//
ENDINGIT

```

Table 4. Carbonation Reactor Data and Calculated Interfacial Areas for Ideal Flow
Calcium Hydroxide Data of Sheppard et al. (15)

Run No.	Impeller Speed (rpm)	Gas Flow Rate (L/min)	Impeller Diameter (cm)	Slurry Density (g/cm ³)	Weight Fraction Solids	Slurry Viscosity (10 ⁻² g/cm-s)	Unagitated Slurry Height (cm)	Agitated Slurry Height (cm)	Decantation Factor	Alpha (cm)	Interfacial Area (cm ² /g)	Interfacial Area (Complete Backmixing) (cm ² /g)
11	350	10.6	12.7	1.038	0.0714	1.210	27.3	28.3	55	7.5237	0.53	7.18
12	450	10.6	12.7	1.038	0.0714	1.210	27.3	29.3	122	7.7895	0.62	15.56
13	550	10.6	12.7	1.038	0.0714	1.210	27.3	30.0	183	7.9756	0.65	22.06
14	650	10.6	12.7	1.038	0.0714	1.210	27.3	30.5	206	8.1086	0.66	25.31
21	350	30.1	12.7	1.038	0.0714	1.210	27.4	28.5	8	2.6683	0.78	2.66
22	450	30.1	12.7	1.038	0.0714	1.210	27.4	29.0	13	2.7151	0.95	4.35
23	550	30.1	12.7	1.038	0.0714	1.210	27.4	30.0	22	2.8087	1.10	7.46
24	650	30.1	12.7	1.038	0.0714	1.210	27.4	31.0	38	2.9023	1.24	12.15
31	350	46.5	12.7	1.038	0.0714	1.210	27.2	28.7	5	1.7393	0.91	2.21
32	450	46.5	12.7	1.038	0.0714	1.210	27.2	29.2	7	1.7696	1.09	3.34
33	550	46.5	12.7	1.038	0.0714	1.210	27.2	30.0	11	1.8181	1.30	5.29
34	650	46.5	12.7	1.038	0.0714	1.210	27.2	31.5	14	1.9090	1.38	6.83
41	350	75.0	12.7	1.038	0.0714	1.210	27.2	29.5	3	1.1094	1.04	1.96
42	450	75.0	12.7	1.038	0.0714	1.210	27.2	30.5	4	1.1272	1.24	2.69
43	550	75.0	12.7	1.038	0.0714	1.210	27.2	30.5	6	1.1660	1.51	4.08
44	650	75.0	12.7	1.038	0.0714	1.210	27.2	31.5	7	1.1825	1.70	5.45
51	350	10.8	12.7	1.018	0.0364	1.099	28.4	29.0	143	7.5670	0.66	18.83
52	450	10.8	12.7	1.018	0.0364	1.099	28.4	29.5	329	7.6875	0.77	42.15
53	550	10.8	12.7	1.018	0.0364	1.099	28.4	30.0	846	7.8279	0.88	107.97
54	650	10.8	12.7	1.018	0.0364	1.099	28.4	30.5	1222	7.8854	0.90	154.97
61	350	31.1	12.7	1.018	0.0364	1.099	28.4	29.8	12	2.7003	0.93	4.21
62	450	31.1	12.7	1.018	0.0364	1.099	28.4	30.2	28	2.7365	1.18	8.98
63	550	31.1	12.7	1.018	0.0364	1.099	28.4	31.0	46	2.8090	1.36	15.96
64	650	31.1	12.7	1.018	0.0364	1.099	28.4	32.0	72	2.8996	1.47	24.40
71	350	46.6	12.7	1.018	0.0364	1.099	28.3	30.5	7	1.8444	1.02	2.99
72	450	46.6	12.7	1.018	0.0364	1.099	28.3	30.5	10	1.8444	1.27	5.10
73	550	46.6	12.7	1.018	0.0364	1.099	28.3	31.2	16	1.8866	1.46	8.04
74	650	46.6	12.7	1.018	0.0364	1.099	28.3	32.0	25	1.9351	1.67	12.60
81	350	75.0	12.7	1.018	0.0364	1.099	27.5	30.0	3	1.1272	1.07	2.08
82	450	75.0	12.7	1.018	0.0364	1.099	27.5	31.0	6	1.1648	1.47	3.90
83	550	75.0	12.7	1.018	0.0364	1.099	27.5	31.5	8	1.1836	1.76	5.97
84	650	75.0	12.7	1.018	0.0364	1.099	27.5	31.5	11	1.1836	2.00	8.27
91	350	10.2	12.7	1.056	0.1056	1.484	27.5	28.5	60	7.8740	0.52	7.49
92	450	10.2	12.7	1.056	0.1056	1.484	27.5	29.0	114	8.0121	0.59	14.08
93	550	10.2	12.7	1.056	0.1056	1.484	27.5	30.0	174	8.2684	0.62	20.83
94	650	10.2	12.7	1.056	0.1056	1.484	27.5	30.5	236	8.4265	0.65	27.85
101	350	31.9	12.7	1.056	0.1056	1.484	27.5	29.3	7	2.5619	0.77	2.44
102	450	31.9	12.7	1.056	0.1056	1.484	27.5	29.5	12	2.6060	0.94	4.09
103	550	31.9	12.7	1.056	0.1056	1.484	27.5	30.5	19	2.6844	1.10	6.83
104	650	31.9	12.7	1.056	0.1056	1.484	27.5	31.0	30	2.7385	1.24	10.39
111	350	46.5	12.7	1.056	0.1056	1.484	27.3	29.0	5	1.7575	0.96	2.50
112	450	46.5	12.7	1.056	0.1056	1.484	27.3	29.7	7	1.7899	1.11	3.87
113	550	46.5	12.7	1.056	0.1056	1.484	27.3	30.5	11	1.8484	1.28	5.22
114	650	46.5	12.7	1.056	0.1056	1.484	27.3	31.5	16	1.9090	1.48	7.79
121	350	75.0	12.7	1.056	0.1056	1.484	27.1	29.5	3	1.1094	0.98	1.68
122	450	75.0	12.7	1.056	0.1056	1.484	27.1	30.0	4	1.1272	1.28	2.86
123	550	75.0	12.7	1.056	0.1056	1.484	27.1	31.0	5	1.1648	1.46	3.82
124	650	75.0	12.7	1.056	0.1056	1.484	27.1	32.0	7	1.2024	1.67	4.68
131	350	10.4	13.7	1.018	0.0364	1.099	27.5	29.2	145	7.6413	0.65	18.89
132	450	10.4	13.7	1.018	0.0364	1.099	27.5	29.2	317	7.9122	0.73	39.98

Table 4 (continued)

Calcium Hydroxide Data (continued)												
Run No.	Impeller Speed (rpm)	Gas Flow Rate (g/min)	Impeller Diameter (cm)	Slurry Density (g/cm ³)	Weight Fraction Solids	Slurry Viscosity (10 ⁻² g/cm-s)	Unagitated Slurry Height (cm)	Agitated Slurry Height (cm)	Decontamination Factor	Alpha (cm)	Interfacial Area (Plug Flow) (cm ² /cm ³)	Interfacial Area (Complete Backmixing) (cm ² /cm ³)
133	550	10.4	13.7	1.018	0.0364	1.099	27.5	29.7	423	8.0477	0.75	52.45
134	650	10.4	13.7	1.018	0.0364	1.099	27.5	30.0	493	8.1290	0.73	60.47
141	350	31.0	13.7	1.018	0.0364	1.099	27.4	28.7	10	2.4509	0.95	3.80
142	450	33.0	13.7	1.018	0.0364	1.099	27.4	29.7	17	2.5362	1.13	6.49
143	550	31.0	13.7	1.018	0.0364	1.099	27.5	30.5	40	2.7726	1.33	13.96
144	650	31.0	13.7	1.018	0.0364	1.099	27.5	31.0	62	2.8181	1.46	21.66
151	450	46.5	13.7	1.018	0.0364	1.099	27.0	29.0	7	1.7575	1.12	3.47
152	550	46.5	13.7	1.018	0.0364	1.099	27.0	29.5	11	1.7878	1.34	5.53
153	650	46.5	13.7	1.018	0.0364	1.099	27.0	30.2	17	1.8202	1.55	8.75
154	650	46.5	13.7	1.018	0.0364	1.099	27.0	31.1	24	1.8648	1.68	12.07
161	350	75.1	13.7	1.018	0.0364	1.099	27.0	30.0	4	1.1257	1.24	2.69
162	450	75.1	13.7	1.018	0.0364	1.099	27.0	30.5	5	1.1465	1.49	3.91
163	550	75.1	13.7	1.018	0.0364	1.099	27.0	31.0	7	1.1632	1.67	5.13
164	650	75.1	13.7	1.018	0.0364	1.099	27.0	32.0	9	1.2008	1.81	6.48
171	350	10.2	13.7	1.038	0.0714	1.210	27.5	28.3	76	7.8187	0.55	9.62
172	450	10.2	13.7	1.038	0.0714	1.210	27.5	29.0	139	8.0121	0.62	17.18
173	550	10.2	13.7	1.038	0.0714	1.210	27.5	30.0	209	8.2884	0.64	25.08
174	650	10.2	13.7	1.038	0.0714	1.210	27.5	30.5	252	8.4255	0.66	29.78
181	350	30.0	13.7	1.038	0.0714	1.210	27.5	28.7	11	2.6959	0.88	3.60
182	450	30.0	13.7	1.038	0.0714	1.210	27.5	29.5	18	2.7711	1.05	6.29
183	550	30.0	13.7	1.038	0.0714	1.210	27.5	30.5	31	2.8650	1.20	10.42
184	650	30.0	13.7	1.038	0.0714	1.210	27.5	31.0	43	2.9120	1.29	14.43
191	350	47.9	13.7	1.038	0.0714	1.210	27.5	29.3	6	1.7238	1.08	3.13
192	450	47.9	13.7	1.038	0.0714	1.210	27.5	30.0	9	1.7650	1.26	4.70
193	550	47.9	13.7	1.038	0.0714	1.210	27.5	30.5	14	1.7944	1.47	7.17
194	650	47.9	13.7	1.038	0.0714	1.210	27.5	31.5	18	1.8532	1.57	9.41
201	350	77.9	13.7	1.038	0.0714	1.210	27.5	29.7	4	1.0744	1.24	2.58
202	450	77.9	13.7	1.038	0.0714	1.210	27.5	30.2	5	1.0825	1.52	3.88
203	550	77.9	13.7	1.038	0.0714	1.210	27.5	31.5	7	1.1395	1.71	5.31
204	650	77.9	13.7	1.038	0.0714	1.210	27.5	32.0	8	1.1576	1.84	6.37
211	350	10.6	13.7	1.056	0.1056	1.484	27.5	28.2	39	7.4971	0.49	5.11
212	450	10.6	13.7	1.056	0.1056	1.484	27.5	29.0	73	7.7098	0.56	9.38
213	550	10.6	13.7	1.056	0.1056	1.484	27.5	29.7	114	7.8959	0.60	14.29
214	650	10.6	13.7	1.056	0.1056	1.484	27.5	30.5	157	8.1086	0.62	19.26
221	350	31.7	13.7	1.056	0.1056	1.484	27.5	28.7	9	2.514	0.84	2.94
222	450	31.7	13.7	1.056	0.1056	1.484	27.5	29.2	13	2.5988	0.99	4.62
223	550	31.7	13.7	1.056	0.1056	1.484	27.5	29.7	21	2.6403	1.15	7.43
224	650	31.7	13.7	1.056	0.1056	1.484	27.5	30.5	28	2.7114	1.23	9.95
231	350	46.5	13.7	1.056	0.1056	1.484	27.5	29.0	6	1.7575	0.98	2.62
232	450	46.5	13.7	1.056	0.1056	1.484	27.5	29.5	8	1.7897	1.15	3.86
233	550	46.5	13.7	1.056	0.1056	1.484	27.5	30.5	12	1.8484	1.33	5.75
234	650	46.5	13.7	1.056	0.1056	1.484	27.5	31.3	15	1.8969	1.43	7.38
241	350	77.9	13.7	1.056	0.1056	1.484	27.5	29.3	3	1.0672	1.09	2.07
242	450	77.9	13.7	1.056	0.1056	1.484	27.5	30.0	5	1.0853	1.41	3.31
243	550	77.9	13.7	1.056	0.1056	1.484	27.5	30.7	6	1.1106	1.57	4.24
244	650	77.9	13.7	1.056	0.1056	1.484	27.5	31.5	7	1.1395	1.70	5.22

Table 4 (continued)

Calcium Hydroxide Data (This Study)												
Pan No.	Impeller Speed (rpm)	Gas Flow Rate (g/min)	Impeller Diameter (cm)	Slurry Density (g/cm ³)	Weight Fraction Solids	Slurry Viscosity (10 ⁻² g/cm-s)	Unagitated Slurry Height (cm)	Agitated Slurry Height (cm)	Decontamination Factor	Alpha (cm)	Interfacial Area (Plug Flow) (cm ² /cm ³)	Interfacial Area (Complete Backmixing) (cm ² /cm ³)
73	350	10.3	13.7	1.038	0.0714	1.210	26.8	28.0	83	7.6682	0.58	10.72
83	350	10.3	13.7	1.038	0.0714	1.210	26.8	28.0	75	7.6682	0.56	9.63
84	450	10.3	13.7	1.038	0.0714	1.210	27.0	28.5	136	7.8051	0.63	17.28
95	550	10.3	13.7	1.038	0.0714	1.210	27.0	29.5	128	8.0790	0.64	21.90
96	650	10.3	13.7	1.038	0.0714	1.210	27.0	30.0	224	8.2159	0.66	27.11
103	350	23.8	13.7	1.038	0.0714	1.210	27.0	28.2	18	3.3461	0.86	4.96
104	450	23.8	13.7	1.038	0.0714	1.210	27.0	29.0	28	3.4410	0.97	7.88
105	550	23.8	13.7	1.038	0.0714	1.210	27.0	29.8	42	3.5356	1.06	11.55
106	650	23.8	13.7	1.038	0.0714	1.210	27.0	30.5	60	3.6190	1.13	16.38
113	350	43.6	13.7	1.038	0.0714	1.210	26.7	28.5	3	1.8438	0.45	2.07
114	450	43.6	13.7	1.038	0.0714	1.210	26.7	29.5	7	1.9085	1.03	3.19
115	550	43.6	13.7	1.038	0.0714	1.210	26.8	30.3	11	1.9602	1.23	5.19
116	650	44.1	13.7	1.038	0.0714	1.210	27.0	30.8	18	1.9668	1.46	8.48
Barium Hydroxide Data (This Study)												
127	250	10.4	13.7	1.121	0.2111	1.200	26.0	27.0	927	14.9209	0.46	62.06
123	350	10.3	13.7	1.121	0.2111	1.200	26.1	28.2	1930	15.7658	0.48	132.34
124	450	10.3	13.7	1.121	0.2111	1.200	26.2	30.0	1817	16.7272	0.45	114.33
125	550	10.3	13.7	1.121	0.2111	1.200	26.3	31.0	1667	17.3312	0.43	96.11
126	650	10.3	13.7	1.121	0.2111	1.200	26.5	31.5	1041	17.6108	0.39	59.06
133	350	23.5	13.7	1.121	0.2111	1.200	26.6	28.2	310	6.9152	0.83	44.62
134	450	23.2	13.7	1.121	0.2111	1.200	26.8	29.8	982	7.3890	0.93	132.60
135	550	23.5	13.7	1.121	0.2111	1.200	26.9	31.0	1022	7.6018	0.91	134.27
136	650	23.5	13.7	1.121	0.2111	1.200	26.0	32.0	930	7.8470	0.87	118.33
143	350	43.6	13.7	1.121	0.2111	1.200	26.2	28.8	60	3.8035	1.08	18.47
144	450	43.6	13.7	1.121	0.2111	1.200	26.3	30.3	225	4.0016	1.35	55.96
145	550	43.6	13.7	1.121	0.2111	1.200	26.5	31.0	508	4.0941	1.57	123.76
146	650	43.6	13.7	1.121	0.2111	1.200	27.0	32.5	222	4.2822	1.24	51.54
153	350	23.5	13.7	1.064	0.1186	1.150	26.4	28.6	222	7.0133	0.77	31.46
154	450	23.5	13.7	1.064	0.1186	1.150	26.5	30.5	620	7.4792	0.86	82.80
155	550	23.5	13.7	1.064	0.1186	1.150	26.6	31.5	943	7.7244	0.89	121.93
156	650	23.5	13.7	1.064	0.1186	1.150	26.9	32.0	446	7.8470	0.78	54.70
182	350	10.3	13.7	1.064	0.1186	1.150	26.8	27.8	946	15.5422	0.44	60.77
183	450	10.3	13.7	1.064	0.1186	1.150	26.8	28.8	1667	16.1013	0.46	103.45
184	550	10.3	13.7	1.064	0.1186	1.150	26.8	30.2	1854	16.6640	0.45	109.75
185	650	10.3	13.7	1.064	0.1186	1.150	26.8	31.2	2075	17.4430	0.44	118.93
186	350	10.3	13.7	1.064	0.1186	1.150	26.7	28.9	2143	17.6108	0.44	121.52
190	350	38.3	13.7	1.064	0.1186	1.150	26.7	28.9	48	4.2359	0.91	11.08
193	350	43.6	13.7	1.064	0.1186	1.150	26.7	28.8	44	3.8038	0.99	11.22
194	450	43.6	13.7	1.064	0.1186	1.150	26.7	30.2	128	3.8084	1.22	31.77
195	550	43.8	13.7	1.064	0.1186	1.150	26.7	31.2	381	4.0942	1.48	92.83
196	650	43.6	13.7	1.064	0.1186	1.150	26.0	32.0	641	4.2262	1.53	151.39

8.4 Location of Original Data

The original data are found in ORNL Databook A-9177-G, pp. 1-31, on file at the MIT School of Chemical Engineering Practice, Bldg. 1505, ORNL.

8.5 Nomenclature

a	gas-liquid interfacial area, cm^2/cm^3
A	contactor cross-sectional area, cm^2
$[\text{CO}_2]$	concentration of CO_2 in liquid, gmol/cm^3
D_{CO_2}	diffusivity of CO_2 in aqueous solution, cm^2/s
DF	decontamination factor (x_0/x_f)
d_I	impeller diameter, cm
G	molar gas flow rate, gmol/s
h	sum of contributions effecting ionic strength [Eq. (19)]
H	Henry's coefficient of solubility, $\text{gmol}/\text{cm}^3\text{-kPa}$
H_0	Henry's coefficient of solubility of CO_2 in pure water, $\text{gmol}/\text{cm}^3\text{-kPa}$
I	ionic strength of the solution
K_1	pseudo-first-order rate constant, $\text{gmol}/\text{cm}^2\text{-kPa-s}$
K_2	second-order rate constant, $\text{cm}^3/\text{gmol-s}$
K_G	gas-side mass transfer coefficient, $\text{gmol}/\text{cm}^2\text{-kPa-s}$
K_L	liquid-side mass transfer coefficient, cm/s
K_R	a lumped reaction constant, $\text{gmol}/\text{cm}^2\text{-s-kPa}$
K°	second-order rate constant in pure water
MW_{air}	molecular weight of air, g/gmol
n	number of equal-volume CSTR's in series
N	impeller speed, rpm
$[\text{OH}^-]$	hydroxide concentration, gmol/cm^3

P	power dissipated per volume of liquid, hp/ft ³
P_{avg}	average pressure in contactor, kPa
P_G	partial pressure of CO ₂ in gas, kPa
P_I	partial pressure of CO ₂ at gas/liquid interface, kPa
Q	air flow rate at STP, l/min
R	specific rate of absorption of CO ₂ , gmol/cm ³ -s
S	weight fraction solids
U	superficial gas velocity, cm/s
U_t	velocity rise of bubbles, cm/s
V_a	aerated volume in contactor, cm ³
x	mole fraction CO ₂ in gas stream
x_f	mole fraction CO ₂ at contactor outlet
x_0	mole fraction CO ₂ at contactor inlet
z	height in contactor, cm
Z_i	valence

Greek Symbols

α	$0.06 \times k_1 P_{avg} V_a M_{air}/Q \rho_{air}$, cm
μ	liquid viscosity, 10 ⁻² g/cm-s
ρ	liquid density, g/cm ³
ρ_{air}	air density, g/cm ³
σ	surface tension, 10 ⁻⁵ J/cm or g/s ²

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